Abstract for Invited Talk

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UNDERSTANDING ADSORBATE STRUCTURES IN FILM GROWTH ON SI(100). Peter J. Bedrossian, Lawrence Livermore National Laboratory, L-350, Livermore, CA 94550

Tailoring thin film microstructure on the atomic level requires control over the occurrence and distribution of interfacial defect structures. The characterization of two interfacial systems on Si(100) illustrates evolving, complimentary insight from modeling and experimental verification.

Both tight-binding and first-principles calculations predict a strong tendency for Mo atoms to adopt high-coordination sites in silicon, which in turn underlies the observed Mo/Si intermixing on Si(100) even for submonolayer Mo deposition. STM and glancing-incidence X-ray diffraction reveal distinct, two-dimensional surface alloys below 650C and disilicide phases in microcrystallites at higher temperatures.

Si atoms also assume a variety of metastable nucleation structures on Si(100). At room temperature, STM reveals Si atoms on top of dimer rows. At slightly higher temperature, "diluted dimers" appear with Si-Si bonds perpendicular to those of familiar Si dimers which form at still higher temperatures. Alternative models of Si adatom nucleation and diffusion may be tested against this observed hierarchy. For thicker Si films or in layer-by-layer removal by sputtering, antiphase boundaries critically affect the occurrence of island nuclei and "solitary dimer rows."

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